Enthalpy and Heat Capacity of Zr-2.5% Nb

Preliminary Recommendation

The preliminary recommendation for the heat capacity and enthalpy of Zr-2.5% Nb in the α-phase are equations obtained from a combined fit of the data from the Chinese Institute of Atomic Energy (CIAE)[1] and the Atomic Energy of Canada Limited (AECL) data reported by Price. [2]
For the α-phase (500-1100 K),

$$C_P\,(J{\cdot}g^{-1}{\cdot}K^{-1}) = 0.2525 + 9.486\,\mathrm{x}\,10^{-5}T \qquad \textbf{(1)}$$

$$H(T) - H(298)\ (kJ{\cdot}kg^{-1}) = -79.46 + 0.2525T + 4.743\,\mathrm{x}\,10^{-5}T^2 \qquad \textbf{(2)}$$

Graphs of the available data and the recommended linear equation for the α-phase heat capacity are shown in Figure 1.

The preliminary recommendation for the β-phase heat capacity is the β-phase heat capacity equation for Zr-1%Nb from measurements by Peletsky and Petrova [3]. It was selected based on agreement of the equation of Pelestky and Petrova [3] with a single available Zr-2.5% Nb heat capacity datum in the β-phase [4]. The corresponding equation for the enthalpy of Zr-2.5% Nb is an estimate obtained from integration of this heat capacity equation with the constant of integration obtained by assuming that the enthalpy of transition for Zr-2.5% Nb is the same as that for Zr-1% Nb.
For the β-phase (1250-2000 K),

$$C_P\,(J{\cdot}g^{-1}{\cdot}K^{-1}) = 0.2813 + 6.625\,\mathrm{x}\,10^{-5}T \qquad \textbf{(3)}$$

$$H(T) - H(298)\ (kJ{\cdot}kg^{-1}) = -42.65 + 0.2813T + 3.313\,\mathrm{x}\,10^{-5}T^2 \qquad \textbf{(4)}$$

The recommended enthalpy increments for Zr-2.5% Nb and Zr-1%Nb are shown in Figure 2. Tabulated values of the heat capacity and enthalpy increments are given in Table 1.

Uncertainty

The errors in fitting the α-phase heat capacity data vary from less than 0.1% to ± 3.6%. These are less than the measurement errors. Thus, the uncertainty for Eqs.(1-2) is 10%, the uncertainty in the measurements. Because the equations for the β-phase are estimates, their uncertainties should be considered to be on the order of 25%.

Discussion

α-phase: Three sets of measurements of the heat capacity of Zr-2.5%Nb alloy that have been reported [1] are shown in Figure 1. The data from the Chinese Institute of Atomic Energy (labeled CIAE in the figures) is in reasonable agreement with the cold-worked and heat-treated AECL data (labeled respectively AECL C1 and AECL H1 in the figures) reported by Price [2]. The AECL data for cold-worked Zr-2.5%Nb (labeled AECL C2 in the figures) reported by Mills et al. [5,1] have not been included in the regression analysis because they are inconsistent with the other available data. Figure 1 shows the recommended heat capacity equation obtained from the regression analysis and the equation for Zr-1%Nb from measurement by Peletsky, Petrova, and Lusternick [3, 6, 7]. Ozrin et al.[8] recommended the heat capacity equation for Zr-1%Nb as an approximation to the heat capacity of Zr-2.5%Nb. Figure 1 shows that it is not a good approximation, particularly at higher temperatures.

The equation for the enthalpy increments of Zr-2.5% Nb, Eq. (2) in the α-phase was obtained by integrating the heat capacity equation with the constant of integration determined by the constraint that the enthalpy increment, H(T)-H(298.15 K), is 0 at T=298.15. The recommended enthalpy increments for Zr-2.5% Nb are shown in Figure 2 and compared with the enthalpy increments for Zr-1%Nb.

β-phase: The only Zr-2.5% Nb data at temperatures above the α-phase are preliminary heat capacity data in the phase transition region and at 1400 K from CIAE measurements that were included in a draft IAEA technical report that was reviewed at an IAEA meeting [4]. Unfortunately, they were not included in the tabulated data given in the final IAEA technical document [1]. The preliminary data are shown in Figure 3 (labeled Chinese Inst. Zr-2.5% Nb) along with the α-phase data from the final IAEA report [1]. Figure 3 shows that the 1400 K β-phase datum is in good agreement with the β-phase heat capacity equation for Zr-1%Nb obtained from measurements by Peletsky and Petrova [3]. Thus, the Zr-1%Nb heat capacity equation of Peletsky and Petrova, Eq. (3), is a reasonable estimate for the β-phase heat capacity of Zr-2.5% Nb.

If the same enthalpy of transition is assumed for Zr-2.5% Nb and Zr-1%Nb, then the estimated equation for the enthalpy increments of Zr-2.5% Nb is identical to that for Zr-1%Nb except for the constant. The constants are different because the α-phase enthalpy increments of Zr-2.5%Nb differ from the α-phase enthalpy increments of Zr-1%Nb. The enthalpy equations for Zr-1%Nb and Zr-2.5% Nb for the α- and β-phases are compared in Figure 2. The enthalpy equations for Zr-1%Nb are from measurements by Peletsky and Petrova [3]. The Zr-1%Nb α-phase equation is identical to that given in 1993 papers by Lusternik, Peletsky, and Petrova. [7,8]

References

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Table 1 Enthalpy and Heat Capacity of Zr-2.5% Nb

Temperature K	H(T)-H(298.15 K) $kJ \cdot kg^{-1}$	Heat Capacity $kJ \cdot kg^{-1} \cdot K^{-1}$
298.15	0.0	281
300	0.6	281
400	29.1	290
500	58.6	300
600	89.1	309
700	121	319
800	153	328
900	186	337
1000	220	347
1100	256	357
1200	343	361
1300	379	367
1400	416	374
1500	454	381
1600	492	387
1700	531	394
1800	571	401
1900	611	407
2000	652	414

Figure 1 Heat Capacity of Zr-2.5% Nb

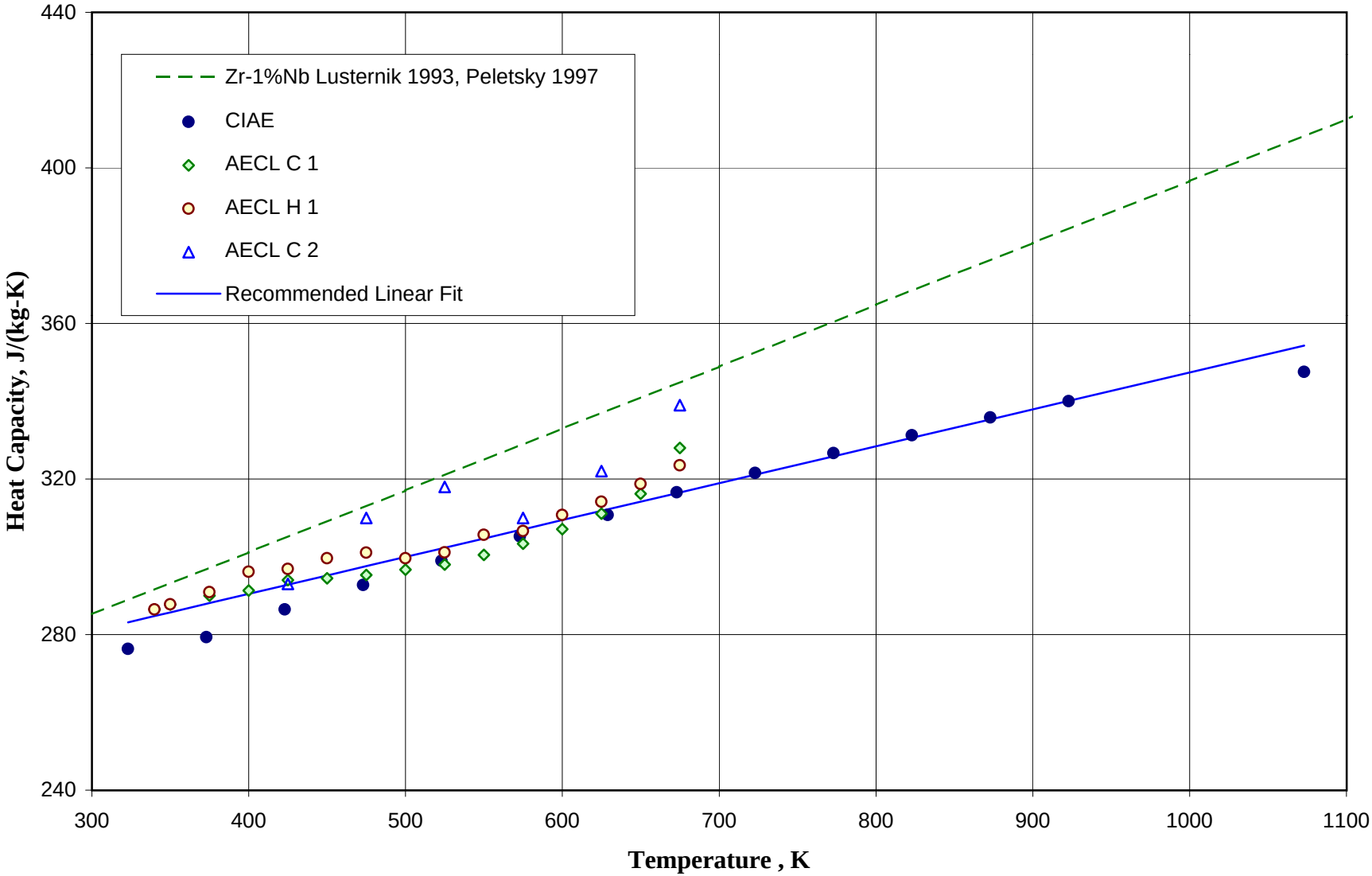

Figure 2 Enthalpy of Zr-Nb

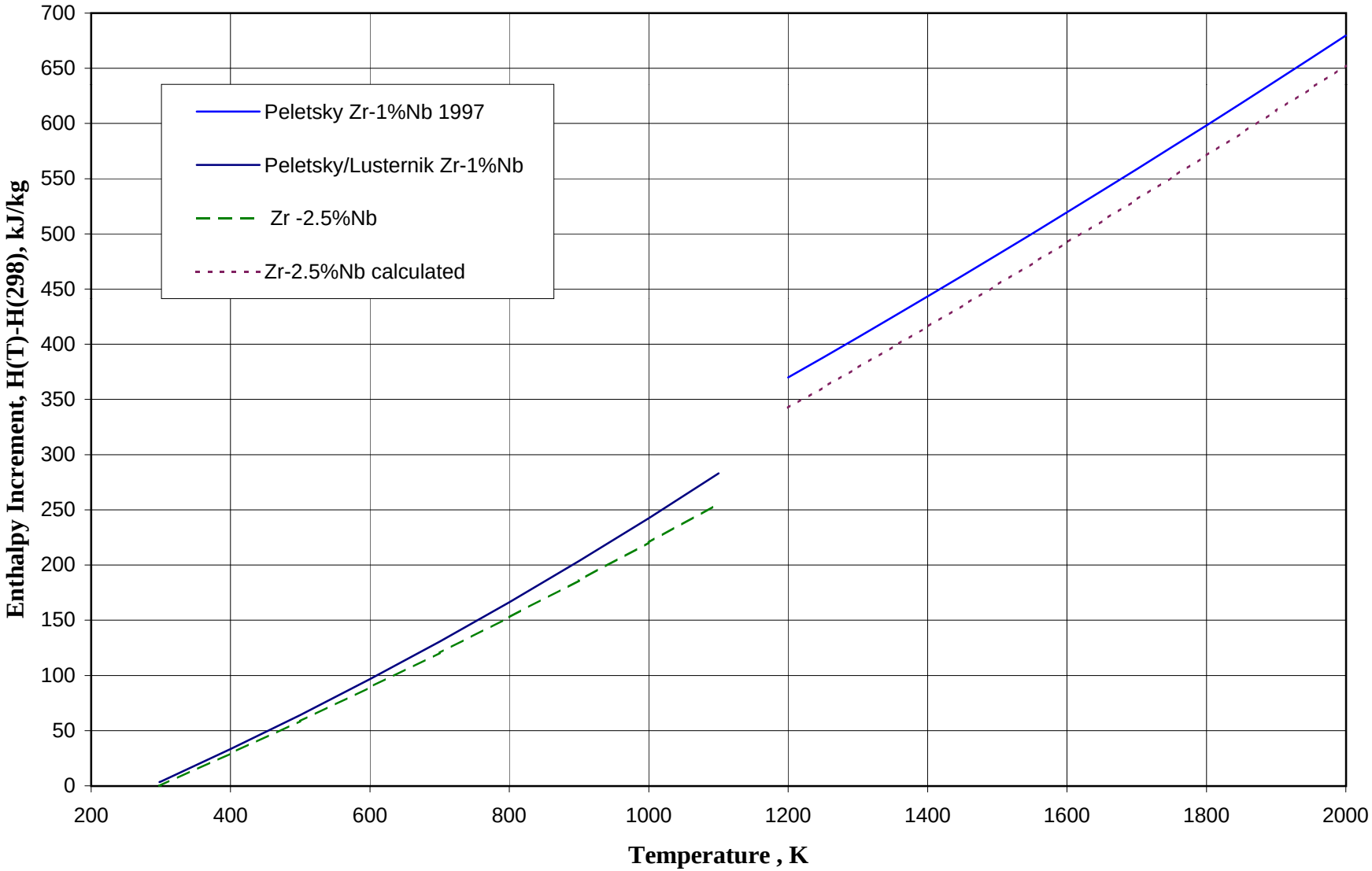

Figure 3 Heat Capacity of Zr-2.5% Nb